# Supporting Information

# Structural Prediction and Multilayer $Li^+$ Storage in Two Dimensional $VC_2$ Carbide Studied by First-Principles Calculations

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**Table S1** Structure parameters of the predicted $VC_2$ monolayers and stacked multilayer.

| | $VC_2$-α | $VC_2$-β | $VC_2$-T | S-$VC_2$ |
|---|---|---|---|---|
| a (Å) | 2.6945 | 3.2769 | 2.9646 | 3.2855 |
| b (Å) | 4.2735 | 4.6232 | 2.9646 | 4.6349 |
| c (Å) | 22.5267 | 22.1872 | 22.0696 | 11.0738 |
| α = β = γ | 90° | 90° | α = β =90°, γ=120° | 90° |
| V-C (Å) | 2.0558/2.1241 | 1.9266/2.1245 | 2.0001 | 1.9305/2.1274 |
| C-C (Å) | 1.3409 | 1.3478 | - | 1.347 |

**Table S2** Adsorption energy ($E_{ad}$) and transferred charges (Δe) per Li atom at different sites with a 3 × 3 × 1 $VC_2$ supercell.

| site | $V_{18}C_{36}Li$-α | | $V_{18}C_{36}Li$-β | |
|---|---|---|---|---|
| | $E_{ad}$ (eV) | Δe-Li | $E_{ad}$ (eV) | Δe-Li |
| 1 | -1.2809 | -0.9087 | -1.8775 | -0.9392 |
| 2 | -1.9523 | -0.9168 | -1.2208 | -0.9147 |
| 3 | -1.194 | -0.9108 | -1.7491 | -0.9277 |
| 4 | -1.4245 | -0.9092 | -1.6274 | -0.9368 |

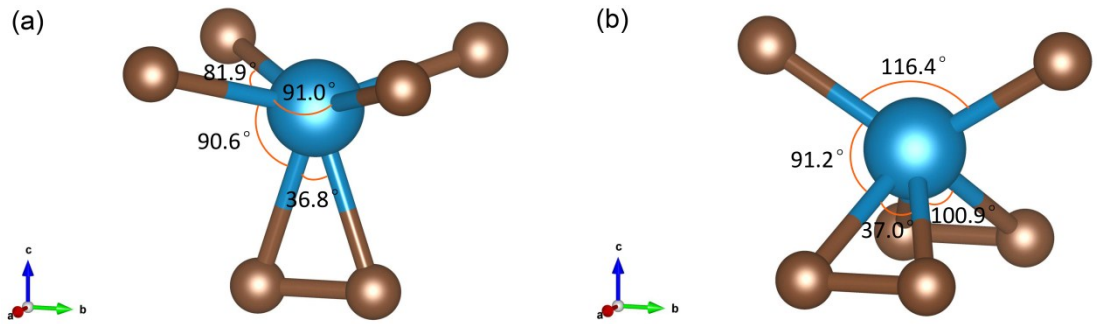


**Fig. S1** Bond angles of C-V-C for (a) $VC_2$-α and (b) $VC_2$-β configurations.

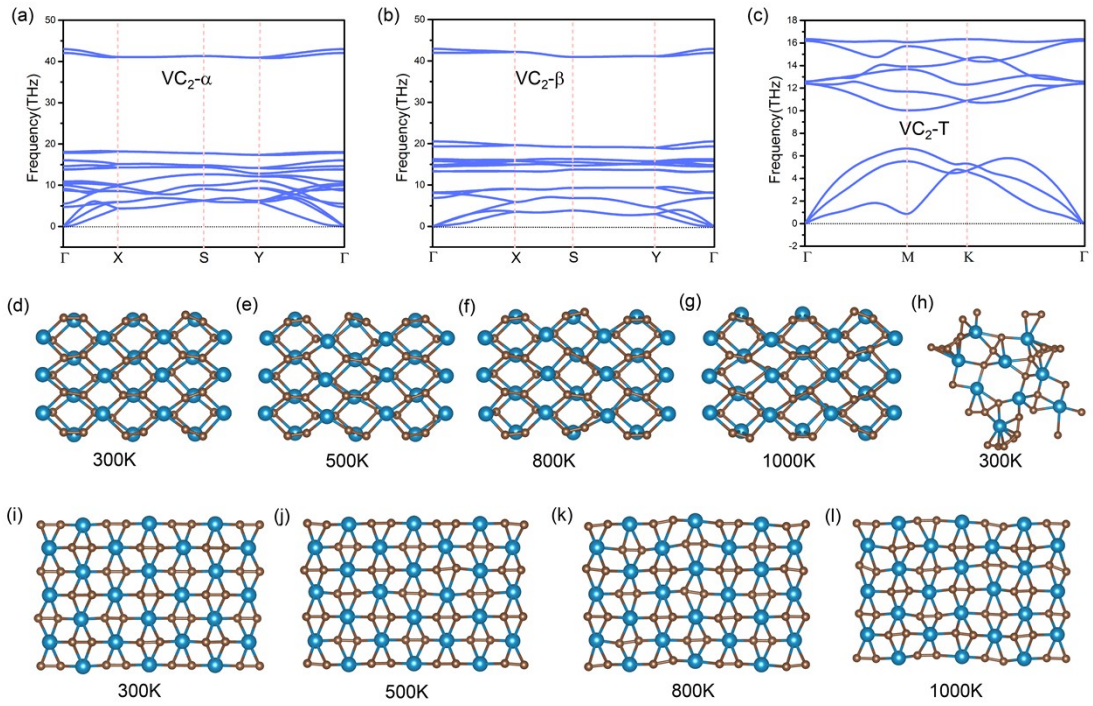


**Fig. S2** Phonon spectra of (a) $VC_2$-α, (b) $VC_2$-β and (c) $VC_2$-T. AIMD simulated $VC_2$ monolayers at 300, 500, 800 and 1000K, (d)-(g) for $VC_2$-α, (h) for $VC_2$-T, and (i)-(l) for $VC_2$-β, respectively.

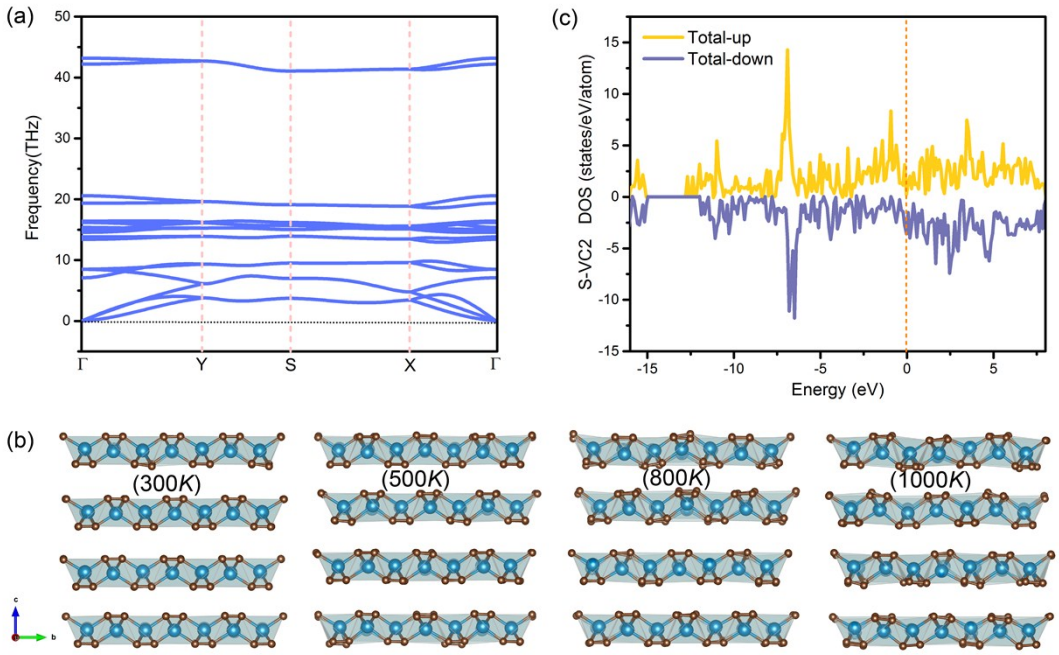


**Fig. S3** (a) phonon spectra, (b) AIMD simulated structures at 300, 500, 800 and 1000K and (c) DOS of S-$VC_2$, respectively.